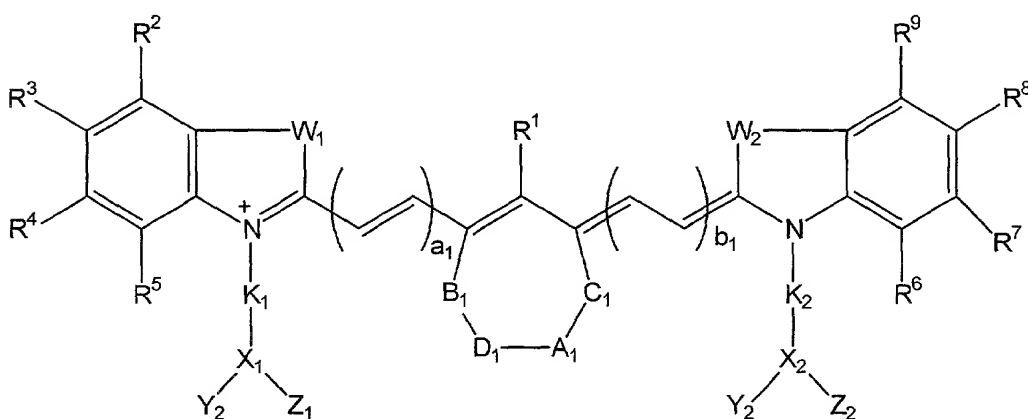


wherein W_1 , W_2 , Y_1 , Y_2 , Z_1 , Z_2 , K_1 , K_2 , Q , X_1 , X_2 , a_1 , and b_1 are defined in the same manner as in Formula 1; and R^{19} to R^{31} are defined in the same manner as R^1 to R^9 in Formula 1.

The invention also relates to the novel composition comprising
5 carbocyanine dyes having a general formula 3



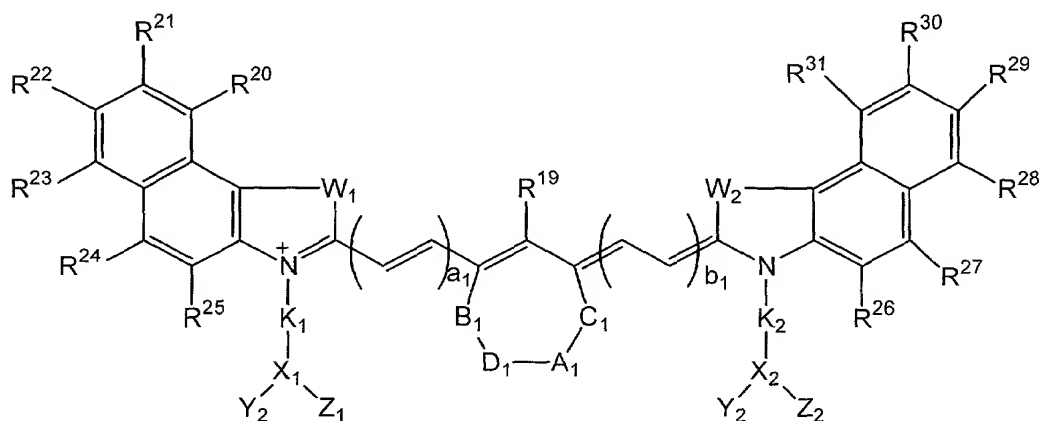
Formula 3

wherein A_1 is a single or a double bond; B_1 , C_1 , and D_1 are independently selected from the group consisting of $-O-$, $-S-$, $-Se-$, $-P-$, $-CR^{10}R^{11}$, $-CR^{11}$, alkyl, NR¹², and $-C=O$; A_1 , B_1 , C_1 , and D_1 may together form a 6- to 12-membered carbocyclic ring or a 6- to 12-membered heterocyclic ring optionally containing
10

one or more oxygen, nitrogen, or sulfur atoms; and W_1 , W_2 , Y_1 , Y_2 , Z_1 , Z_2 , K_1 , K_2 , X_1 , X_2 , a_1 , b_1 , and R^1 to R^{12} are defined in the same manner as in Formula 1.

The present invention also relates to the novel composition comprising carbocyanine dyes having a general formula 4

5



Formula 4

wherein A_1 , B_1 , C_1 , and D_1 are defined in the same manner as in Formula 3; W_1 , W_2 , Y_1 , Y_2 , Z_1 , Z_2 , K_1 , K_2 , X_1 , X_2 , a_1 , and b_1 are defined in the same manner as in Formula 1; and R^{19} to R^{31} are defined in the same manner as R^1 to R^9 in

10 Formula 1.

The inventive bioconjugates use the multiple attachment points of carbocyanine dye structures to incorporate one or more receptor targeting

and/or photosensitive groups in the same molecule. More specifically, the inventive compositions consist of three components selected for their specific properties. One component, a tumor specific agent, is for targeting tumors. A second component, which may be a photosensitizer, is a phototherapy agent.

5 A third component is a photodiagnostic agent.

Examples of the tumor targeting agents are bioactive peptides such as octreotate and bombesin (7-14) which target overexpressed receptors in neuroendocrine tumors. An example of a phototherapy agent is 2-[1-hexyloxyethyl]-2-devinylpyro-pheophorbide-a (HPPH, Figure 1D, T=OH).

10 Examples of photodiagnostic agents are carbocyanine dyes which have high infrared molar absorptivities (Figure 1A-C). The invention provides each of these components, with their associated benefits, in one molecule for an optimum effect.

Such small dye biomolecule conjugates have several advantages
15 over either nonspecific dyes or the conjugation of probes or photosensitive molecules to large biomolecules. These conjugates have enhanced localization and rapid visualization of tumors which is beneficial for both diagnosis and therapy. The agents are rapidly cleared from blood and non-target tissues so there is less concern for accumulation and for toxicity. A
20 variety of high purity compounds may be easily synthesized for combinatorial screening of new targets, e.g., to identify receptors or targeting agents, and for the ability to affect the pharmacokinetics of the conjugates by minor structural changes.

The inventive compositions are useful for various biomedical
25 applications. Examples of these applications include, but are not limited to: